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IONIZATION POTENTIALS, EXPERIMENTAL AND THEORETICAL, OF THE ELEMENTS HYDROGEN TO KRYPTON

by

Raymond L. Kelly and Don E. Harrison, Jr.

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Rear Admiral R. W. McNitt, USN
Superintendent

R. F. Rinehart
Academic Dean

TITLE:

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ABSTRACT:

The ionization potentials of the isoelectronic sequences Helium through Zinc have been calculated by the Hartree-Fock method and compared with experimental results. Tables are presented showing the ionization potentials, as observed and extrapolated, for all stages of ionization of the first 36 elements.

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Because many of the ionization potentials of the lighter elements have not been measured, a number of investigators[1,2,3] have attempted to determine these potentials by interpolation and extrapolation from the available data. These efforts have generally taken the form of extrapolation along isoelectronic sequences through screening number analysis.

The most extensive recent compilation of ionization potentials is that of Lotz[2], who presented results through the 26th spectrum of Zinc (Z=30). His extrapolations were based on the expression

$$T \approx \sum_{n=0}^{4} A_n \zeta^n + C(\zeta+B)^{-1}$$

where ζ is the spectrum number. The A_n, B and C are constants within a sequence. Lotz fitted the experimental data to this formula, and he also included the type of relativistic correction suggested by Edlén[1].

Here we undertake the same type of analysis, basing the extrapolation upon calculated approximations to the ionization potentials. The differences between the theoretical and experimental values are extrapolated, rather than the experimental data themselves. Because we extrapolate relatively small corrections to the theoretical values, the predicted ionization potentials should be quite reliable.

A number of computer programs now exist which will solve the radial portion of the Schrödinger equation for an atom or ion in the Hartree-Fock approximation. The most readily accessible of these are the Herman-Skillman[4] (HS) and the Charlotte Froese Fischer (CFF) programs[5]. We have used these programs to compute ionization potentials for all states of ionization (except for the Hydrogen-

like ions) for the elements from Helium to Zinc. The resulting values were compared against each other and against the experimental values. Where sufficient experimental data exist, the differences between calculated and experimental values were fitted to a second-order polynomial. This difference polynomial provides a reasonable extrapolation formula.

Any calculation of this type must inevitably involve a compromise between computer running time and the level of sophistication of the theoretical model. The Herman-Skillman program was chosen because it runs rapidly and requires a bare minimum of starting parameters. The resultant energy levels E(HS) are the Hartree-Fock-Slater levels to the center of gravity of the ground state of the specified configuration. Ionization potentials calculated with this program usually deviate significantly from the experimental values, but the deviations are completely systematic along an isoelectronic sequence if the configuration does not change. Plausible extrapolations of the difference Δ_{HS}=E(HS) - E(EXPT) can be made for all the systems studied.

The Charlotte Froese Fischer program is much more difficult to use. The stability of the numerical system is uncertain enough that the starting parameters must be adjusted by trial and error until self-consistent solutions finally result.[5] However, because this program includes the electrostatic interactions between electrons through the Slater F^k and G^k integrals, the calculated ionization potentials E(CFF) generally exhibit much better agreement with experiment than do the E(HS) values. The extrapolated quantities Δ_{CFF}=E(CFF) - E(EXPT) are small, so these calculations can be used to predict ionization potentials with a confidence level of better than $\pm$ 0.3%.

The following tables present the data in summary form, the experimental values being derived from spectroscopic publications [2,6,7]. In general, the criterion used in accepting numbers to fill the tables was that the empirically corrected values of the CFF and the HS calculations should agree. This criterion seems plausible, since the two calculations require different corrections and the corrections are frequently of opposite sign.

In the absence of a clear-cut relativistic contribution, the numbers given are basically non-relativistic. For a few cases, Edlén[1] indicates a possible relativistic correction. These have been included for the isoelectronic sequences of Helium, Lithium, Beryllium, Boron, Carbon and Sodium, as indicated in the comments below.

H Sequence:

Precise calculations have been carried out by Garcia and Mack[4] out to Z=20. Extrapolation to higher values of Z was accomplished by fitting the calculated values to a fourth-order polynomial, leading to the following formula:

$$T=(1.85097\times10^{-4})(Z-0.41602)^4+13.6063Z^2-(4.58298\times10^{-3})Z-0.0032$$

Spectrum	I. P.
H I	13.598 eV
He II	54.416
Li III	122.451
Be IV	217.713
B V	340.217
C VI	489.983
N VII	667.029
O VIII	871.390
F IX	1103.09
Ne X	1362.16
Na XI	1648.66
Mg XII	1962.61
Al XIII	2304.08
Si XIV	2673.11
P XV	3069.76
S XVI	3494.10
Cl XVII	3946.19
Ar XVIII	4426.11
K XIX	4933.93
Ca XX	5469.74
Sc XXI	[6033.6]
Ti XXII	[6625.6]
V XXIII	[7245.9]
Cr XXIV	[7894.5]
Mn XXV	[8571.5]
Fe XXVI	[9277.2]
Co XXVII	[10011]
Ni XXVIII	[10775]
Cu XXIX	[11566]
Zn XXX	[12387]
Ga XXXI	[13238]
Ge XXXII	[14117]
As XXXIII	[15026]
Se XXXIV	[15964]
Br XXXV	[16933]
Kr XXXVI	[17931]

He Sequence:

We used the relativistic correction proposed by Edlén[1], $\Delta_R=(1.8112\times10^{-4})\zeta^4$ where the spectrum number $\zeta=Z-1$. When this correction was subtracted from the experimental results, the resulting reduced values fit very well to $T_N=13.6002\zeta^2+10.2436\zeta+0.74314$ or to an Edlén type formula as used by Lotz. (The ionization potential of H^- is thus calculated to be 0.743 eV, compared with the accurate value of 0.755.) The CFF values are almost exactly the same as the reduced values T_N. The final formula is:

$$T=(1.8112\times10^{-4})\zeta^4+13.6002\zeta^2+10.2436\zeta+0.74314.$$

Spectrum	E(EXPT)	Uncorrected E(CFF)	Δ_R	I. P.
He I	24.587 eV	24.978 eV	0 eV	24.587 eV
Li II	75.638	75.980	0.003	75.638
Be III	153.89	154.202	.015	153.89
B IV	259.36	259.637	.046	259.36
C V	392.08	392.283	.113	392.08
N VI	552.06	552.141	.235	552.06
O VII	739.30	739.208	.435	739.30
F VIII	954.84	953.486	.742	953.84
Ne IX	1196	1194.97	1.19	1195.73
Na X	1465	1463.67	1.81	1465.00
Mg XI	1761.7	1759.58	2.65	1761.70
Al XII	2086.0	2082.70	3.78	2085.85
Si XIII		2433.03	5.17	[2438]
P XIV		2810.57	6.96	[2817]
S XV		3215.31	9.17	[3224]
Cl XVI		3647.27	11.87	[3658]
Ar XVII		4106.44	15.13	[4120]
K XVIII		4592.82	19.01	[4611]
Ca XIX		5106.41	23.60	[5129]
Sc XX		5647.21	28.98	[5675]
Ti XXI		6215.22	35.22	[6249]
V XXII		6810.43	42.43	[6851]
Cr XXIII		7432.86	50.68	[7482]
Mn XXIV		8082.50	60.09	[8141]
Fe XXV		8759.35	70.75	[8828]
Co XXVI		9463.41	82.77	[9544]
Ni XXVII		10194.7	96.3	[10288]
Cu XXVIII		10953.2	111.3	[11062]
Zn XXIX		11738.8	128.1	[11864]
Ga XXX		12561.7	146.7	[12695]
Ge XXXI		13391.8	167.3	[13556]
As XXXII		14259.2	189.9	[14445]
Se XXXIII		15153.7	214.8	[15365]
Br XXXIV		16075.4	242.0	[16313]
Kr XXXV		17024.4	271.8	[17292]

Li Sequence:

The data fit well when the Edlén relativistic correction is used. The final formula is (with $\zeta = Z-2$):

$$T = 3.39472 \left[\frac{\zeta^3 + 1.26876^2 - 0.12553\,\zeta + 0.15793}{\zeta + 0.4229} \right] + (5.66 \times 10^{-5})(\zeta + 1)^4$$

Spectrum	E(EXPT)	Uncorrected E(CFF)	Δ_R	I. P.
Li I	5.390 eV	5.342 eV	0 eV	5.390 eV
Be II	18.211	18.126	0.005	18.211
B III	37.930	37.818	.014	37.930
C IV	64.492	64.352	.035	64.492
N V	97.888	97.707	.073	97.888
O VI	138.115	137.876	.136	138.115
F VII	185.185	184.854	.232	185.185
Ne VIII	239.1	238.64	.37	239.10
Na IX	299.85	299.23	.57	299.85
Mg X	367.46	366.62	.83	367.46
Al XI	442.0	440.82	1.17	442.00
Si XII	523.38	521.82	1.62	523.38
P XIII	611.60	609.63	2.17	611.60
S XIV	804.6?	704.24	2.86	[707]
Cl XV		805.65	3.71	[809]
Ar XVI		913.87	4.73	[918]
K XVII		1028.89	5.94	[1034]
Ca XVIII		1150.71	7.38	[1157]
Sc XIX		1279.33	9.06	[1288]
Ti XX		1414.76	11.01	[1425]
V XXI		1556.99	13.26	[1569]
Cr XXII		1706.02	15.84	[1720]
Mm XXIII		1861.86	18.78	[1879]
Fe XXIV		2024.50	22.11	[2045]
Co XXV		2193.94	25.86	[2218]
Ni XXVI		2370.18	30.08	[2398]
Cu XXVII		2553.22	34.79	[2585]
Zn XXVIII		2743.07	40.03	[2780]
Ga XXIX		2939.72	45.84	[2982]
Ge XXX		3143.18	52.27	[3192]
As XXXI		3353.43	59.35	[3409]
Se XXXII		3570.49	67.12	[3633]
Br XXXIII		3794.35	75.63	[3865]
Kr XXXIV		4025.02	84.93	[4105]

Be Sequence:

The non-relativistic extrapolated values are the CFF energies with a ζ^2 correction subtracted.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
Be I	9.322 eV	8.415 eV	9.322 eV
B II	25.155	23.777	25.155
C III	47.883	46.095	47.883
N IV	77.471	75.283	77.471
O V	113.896	111.309	113.896
F VI	157.156	154.158	157.156
Ne VII	207.3	203.82	207.27
Na VIII	264.22	260.30	264.22
Mg IX	327.98	323.58	327.98
Al X	398.6	393.68	398.6
Si XI	476.15	470.58	476.15
P XII	560.5	554.28	560.5
X XIII		644.79	(652)
Cl XIV		742.10	(749)
Ar XV		846.22	(854)
K XVI		957.14	(966)
Ca XVII		1074.9	(1084)
Sc XVIII		1199.4	(1209)
Ti XIX		1330.7	(1342)
V XX		1468.9	(1480)
Cr XXI		1613.8	(1626)
Mn XXII		1765.5	(1779)
Fe XXIII		1924.1	(1938)
Co XXIV		2089.4	(2104)
Ni XXV		2261.6	(2277)
Cu XXVI		2440.5	(2457)
Zn XXVII		2626.3	(2644)
Ga XXVIII		2818.8	(2837)
Ge XXIX		3018.2	(3038)
As XXX		3224.4	(3245)
Se XXXI		3437.3	(3459)
Br XXXII		3657.1	(3680)
Kr XXXIII		3883.7	(3907)

B Sequence:

The non-relativistic extrapolated values are the CFF energies as calculated.

Spectrum	E(EXPT)	Uncorrected E(CFF)
B I	8.298 eV	8.431 eV
C II	24.382	24.618
N III	47.438	47.770
O IV	77.412	77.815
F V	114.24	114.72
Ne VI	157.95	158.45
Na VII	208.50	209.02
Mg VIII	266.02	266.40
Al IX	330.2	330.60
Si X	401.38	401.61
P XI	479.5	479.44
S XII		(564)
Cl XIII		(656)
Ar XIV		(754)
K XV		(859)
Ca XVI		(971)
Sc XVII		(1089)
Ti XVIII		(1215)
V XIX		(1347)
Cr XX		(1486)
Mn XXI		(1632)
Fe XXII		(1784)
Co XXIII		(1944)
Ni XXIV		(2110)
Cu XXV		(2284)
Zn XXVI		(2463)
Ga XXVII		(2650)
Ge XXVIII		(2844)
As XXIX		(3044)
Se XXX		(3251)
Br XXXI		(3465)
Kr XXXII		(3686)

C Sequence:

The non-relativistic extrapolated values are the CFF energies with a ζ^2 correction subtracted.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
C I	11.260 eV	11.791 eV	11.260 eV
N II	29.600	30.206	29.600
O III	54.900	55.614	54.900
F IV	87.16	87.93	87.16
Ne V	126.29	127.12	126.29
Na VI	172.14	173.15	172.14
Mg VII	224.95	226.02	224.95
Al VIII	284.6	285.71	284.6
Si IX	351.05	352.22	351.05
P X	424.4	425.54	424.4
S XI		505.7	(504)
Cl XII		592.6	(591)
Ar XIII		686.4	(685)
K XIV		787.0	(785)
Ca XV		894.3	(893)
Sc XVI		1009	(1007)
Ti XVII		1130	(1128)
V XVIII		1257	(1255)
Cr XIX		1392	(1390)
Mn XX		1533	(1531)
Fe XXI		1682	(1679)
Co XXII		1837	(1834)
Ni XXIII		1998	(1996)
Cu XXIV		2167	(2165)
Zn XXV		2342	(2340)
Ga XXVI		2525	(2522)
Ge XXVII		2714	(2711)
As XXVIII		2909	(2907)
Se XXIX		3112	(3109)
Br XXX		3322	(3319)
Kr XXXI		3538	(3535)

N Sequence:

The non-relativistic extrapolated values are the CFF energies with a ζ^2 correction subtracted.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
N I	14.532 eV	15.444 eV	14.532 eV
O II	35.117	36.105	35.117
F III	62.66	63.776	62.66
Ne IV	97.05	98.37	97.05
Na V	138.40	139.84	138.40
Mg VI	186.54	188.16	186.54
Al VII	241.40	243.33	241.40
Si VIII	303.15	305.32	303.15
P IX	371.6	374.14	371.6
S X	447.1	449.78	447.1
Cl XI	529.3	532.24	529.2
Ar XII	618.5	621.5	618.1
K XIII		717.6	(714)
Ca XIV		820.5	(816)
Sc XV		930.2	(926)
Ti XVI		1047	(1042)
V XVII		1170	(1165)
Cr XVIII		1300	(1295)
Mn XIX		1437	(1431)
Fe XX		1581	(1574)
Co XXI		1731	(1724)
Ni XXII		1889	(1881)
Cu XXIII		2053	(2045)
Zn XXIV		2224	(2215)
Ga XXV		2401	(2392)
Ge XXVI		2586	(2576)
As XXVII		2777	(2767)
Se XXVIII		2976	(2964)
Br XXIX		3181	(3169)
Kr XXX		3392	(3380)

O Sequence:

The non-relativistic extrapolated values are the CFF energies with a ζ^2 correction subtracted.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
O I	13.618 eV	17.194 eV	13.618 eV
F II	34.970	39.295	34.970
Ne III	63.74	68.459	63.74
Na IV	98.905	104.573	98.905
Mg V	141.27	147.58	141.27
Al VI	190.5	197.46	190.5
Si VII	246.5	254.20	246.5
P VIII	309.3	317.76	309.3
S IX	379.05	388.16	379.05
Cl X	455.4	465.38	455.4
Ar XI	539.0	549.43	538.8
K XII		640.3	(629)
Ca XIII		738.0	(726)
Sc XIV		842.4	(830)
Ti XV		953.7	(940)
V XVI		1072	(1058)
Cr XVII		1197	(1182)
Mn XVIII		1328	(1313)
Fe XIX		1467	(1451)
Co XX		1612	(1596)
Ni XXI		1764	(1747)
Cu XXII		1923	(1905)
Zn XXIII		2089	(2070)
Ga XXIV		2262	(2242)
Ge XXV		2441	(2421)
As XXVI		2627	(2606)
Se XXVII		2820	(2798)
Br XXVIII		3020	(2997
Kr XXIX		3227	(3203)

F Sequence:

The non-relativistic extrapolated values are the CFF energies with a ζ^2 correction subtracted.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
F I	17.422 eV	19.864 eV	17.422 eV
Ne II	40.962	43.716	40.962
Na III	71.665	74.671	71.665
Mg IV	109.32	112.60	109.32
Al V	153.8	157.44	153.8
Si VI	205.16	209.17	205.16
P VII	263.37	267.75	263.37
S VIII	328.89	333.18	328.89
Cl IX	400.8	405.44	400.8
Ar X	479.1	484.54	479.6
K XI		570.46	(565)
Ca XII	655 ?	663.20	(657)
Sc XIII		762.8	(756)
Ti XIV		869.1	(862)
V XV		982.3	(975)
Cr XVI		1102	(1095)
Mn XVII		1229	(1222)
Fe XVIII		1362	(1355)
Co XIX		1503	(1495)
Ni XX		1650	(1642)
Cu XXI		1804	(1796)
Zn XXII		1965	(1956)
Ga XXIII		2133	(2123)
Ge XXIV		2307	(2297)
As XXV		2489	(2478)
Se XXVI		2677	(2666)
Br XXVII		2872	(2860)
Kr XXVIII		3073	(3061)

Ne Sequence:

The non-relativistic extrapolated values (beyond Zn XXI) are the CFF energies with a ζ^2 correction added.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
Ne I	21.564 eV	23.140 eV	21.564 eV
Na II	47.302	48.901	47.302
Mg III	80.137	81.798	80.137
Al IV	119.99	121.69	119.99
Si V	166.77	168.51	166.77
P VI	220.47	222.22	220.47
S VII	281.06	282.80	281.06
Cl VIII	348.4	350.23	348.4
Ar IX	422.8	424.51	422.8
K X	503.8	505.61	503.8
Ca XI	591.8	593.55	591.8
Sc XII	686.6	688.31	686.6
Ti XIII	788.4	789.89	788.4
V XIV	897.1	898.28	897.1
Cr XV	1013.0	1013.5	1013.0
Mn XVI	1135.9	1135.5	1135.9
Fe XVII	1266	1264.4	1266.7
Co XVIII	1403	1400.0	1403.4
Ni XIX	1546.9	1542.5	1546.9
Cu XX	1697.9	1691.7	1697.9
Zn XXI	1855.9	1847.8	1855.9
Ga XXII		2011	(2019)
Ge XXIII		2180	(2191)
As XXIV		2356	(2369)
Se XXV		2540	(2554)
Br XXVI		2730	(2746)
Kr XXVII		2927	(2945)

Na Sequence:

We used the Edlén relativistic correction $\Delta_R = (2.012\times10^{-5})\,(\zeta+5)^4$. The final extrapolation formula is (with $\zeta = Z-10$):

$$T = 1.51719\left[\frac{\zeta^3 + 6.4304\zeta^2 + 4.1064\zeta - 0.9786}{\zeta + 2.1434}\right] + (2.012\times10^{-5})\,(\zeta+5)^4$$

Small corrections to the observed values were made at Cl VII, K IX, Ni XVIII, Cu XIX, Zn XX. These are marked by underlining the corrected portion.

Spectrum	E(EXPT)	Uncorrected E(CFF)	Δ_R	I. P.
Na I	5.138 eV	4.955 eV	0.026 eV	5.138 eV
Mg II	15.035	14.733	.048	15.035
Al III	28.447	28.055	.082	28.447
Si IV	45.141	44.664	.132	45.141
P V	65.023	64.454	.201	65.023
S VI	88.051	87.373	.295	88.051
Cl VII	114.30	113.39	.417	114.<u>22</u>
Ar VIII	143.50	142.48	.575	143.50
K IX	175.782	174.65	.773	175.84
Ca X	211.269	209.86	1.018	211.269
Sc XI	249.86	248.13	1.319	249.86
Ti XII	291.545	289.44	1.680	291.545
V XIII	336.377	333.79	2.112	336.377
Cr XIV	384.295	381.18	2.622	384.295
Mn XV	435.323	431.61	3.219	435.323
Fe XVI	489.457	485.06	3.913	489.457
Co XVII	546.816	541.56	4.713	546.816
Ni XVIII	607.18	601.08	5.63	607.<u>30</u>
Cu XIX	670	663.63	6.68	670.<u>95</u>
Zn XX	737.9	729.22	7.86	737.<u>77</u>
Ga XXI		797.83	9.19	[808]
Ge XXII		869.46	10.69	[881]
As XXIII		944.13	12.37	[953]
Se XXIV		1021.8	14.23	[1037]
Br XXV		1102.5	16.30	[1120]
Kr XXVI		1186.3	18.58	[1206]

Mg Sequence:

The non-relativistic extrapolated values (beyond Co XVI) are the CFF energies with a ζ^2 correction added.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
Mg I	7.646 eV	6.886 eV	7.646 eV
Al II	18.828	17.749	18.828
Si III	33.492	32.161	33.492
P IV	51.367	49.881	51.505
S V	72.49	70.800	72.49
Cl VI	97	94.863	96.85
Ar VII	124.03	122.03	124.03
K VIII	155	152.29	154.8
Ca IX	188.0	185.62	188.5
Sc X	225.5	222.01	225.5
Ti XI	265.6	261.46	265.6
V XII	308.0	303.96	308.5
Cr XIII	354.8	349.49	354.8
Mn XIV	404.1	398.07	404.1
Fe XV	456.7	449.69	456.7
Co XVI	512.4	504.34	512.4
Ni XVII		562.03	(571)
Cu XVIII		622.75	(632)
Zn XIX		686.51	(697)
Ga XX		753.29	(765)
Ge XXI		823.10	(836)
As XXII		895.94	(910)
Se XXIII		971.81	(987)
Br XXIV		1050.7	(1067)
Kr XXV		1132.6	(1150)

Al Sequence:

The non-relativistic extrapolated values (beyond Ar VI) are the CFF energies with a ζ^2 correction added.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
Al I	5.986 eV	5.713 eV	5.986 eV
Si II	16.346	15.492	16.346
P III	30.163	29.671	30.163
S IV	47.304	46.711	47.304
Cl V	67.8	66.964	67.8
Ar VI	91.32	90.372	91.32
K VII	118 ?	116.90	(120)
Ca VIII	147 ?	146.53	(150)
Sc IX	180 ?	179.24	(183)
Ti X		215.01	(220)
V XI		253.85	(259)
Cr XII		295.74	(301)
Mn XIII		390.68	(347)
Fe XIV	390 ?	388.66	(395)
Co XV		439.69	(446)
Ni XVI		493.75	(500)
Cu XVII		550.85	(556)
Zn XVIII		610.99	(616)
Ga XIX		674.16	(679)
Ge XX		740.36	(744)
As XXI		809.59	(812)
Se XXII		881.86	(883)
Br XXIII		957.15	(957)
Kr XXIV		1035.5	(1034)

Si Sequence:

The non-relativistic extrapolated values (beyond K VI, but with observations at Fe XIII and Ni XV) are the CFF energies with a ζ^2 correction subtracted.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
Si I	8.151 eV	8.084 eV	8.151 eV
P II	19.73	19.591	19.73
S III	35.06	34.566	35.06
Cl IV	53.46	52.840	53.46
Ar V	75.02	74.322	75.02
K VI	99.74	98.96	99.74
Ca VII	128 ?	126.72	(127.3)
Sc VIII	159 ?	157.58	(157.9)
Ti IX	193 ?	191.52	(191.4)
V X		228.54	(228)
Cr XI		268.61	(267)
Mn XII		311.74	(310)
Fe XIII	355 ?	357.93	355.5
Co XIV		407.15	(404)
Ni XV	455 ?	459.42	455.3
Cu XVI		514.74	(510)
Zn XVII		573.08	(567)
Ga XVIII		634.47	(627)
Ge XIX		698.89	(690)
As XX		766.34	(756)
Se XXI		836.83	(825)
Br XXII		910.34	(897)
Kr XXIII		986.89	(971)

P Sequence:

The non-relativistic extrapolated values are the uncorrected CFF energies, because of the small number of observations.

Spectrum	E(EXPT)	E(CFF)
P I	10.486 eV	10.658 eV
S II	23.411	23.449
Cl III	39.914	39.677
Ar IV	58.81	59.19
K V		81.9
Ca VI		108
Sc VII		137
Ti VIII		169
V IX		204
Cr X		242
Mn XI		283
Fe XII		328
Co XIII		375
Ni XIV		426
Cu XV		479
Zn XVI		536
Ga XVII		596
Ge XVIII		658
As XIX		724
Se XX		793
Br XXI		864
Kr XXII		939

S Sequence:

The non-relativistic extrapolated values (beyond Mn X) are the CFF energies with a ζ^2 correction subtracted.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
S I	10.360 eV	11.901 eV	10.360 eV
Cl II	23.8	25.544	23.8
Ar III	40.909	42.643	40.909
K IV	60.90	63.042	60.90
Ca V	84.41	86.66	84.41
Sc VI	111.1	113.4	111.1
Ti VII	140.8	143.3	140.8
V VIII	173.7	176.4	173.7
Cr IX	209.6	212.5	209.6
Mn X	248	251.6	248.3
Fe XI	290 ?	293.9	(290.2)
Co XII		339	(335)
Ni XIII		388	(383)
Cu XIV		439	(434)
Zn XV		493	(489)
Ga XVI		551	(546)
Ge XVII		611	(606)
As XVIII		675	(669)
Se XIX		742	(735)
Br XX		811	(804)
Kr XXI		884	(876)

Cl Sequence:

The non-relativistic extrapolated values (beyond Co XI) are the uncorrected CFF energies. The corrections Δ_{CFF} are quite small.

Spectrum	E(EXPT)	E(CFF)
Cl I	12.967 eV	13.779 eV
Ar II	27.629	28.444
K III	46.5	46.56
Ca IV	67.9	67.99
Sc V	92.5	92.64
Ti VI	119.5	120.4
V VII	$151.\underline{4}$	151.4
Cr VIII	$185.\underline{4}$	185.4
Mn IX	$222.\underline{6}$	222.6
Fe X	$262.\underline{8}$	262.8
Co XI	305 ?	306.1
Ni XII	350 ?	352.5
Cu XIII		402
Zn XIV		454
Ga XV		510
Ge XVI		568
As XVII		630
Se XVIII		695
Br XIX		762
Kr XX		833

Ar Sequence:

The non-relativistic extrapolated values (beyond Fe IX) are the CFF energies with a ζ^2 correction added.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
Ar I	15.759 eV	16.082 eV	15.759 eV
K II	31.82	31.851	31.82
Ca III	50.908	51.069	50.908
Sc IV	73.9	73.592	73.9
Ti V	99.265	99.338	99.265
V VI	128.9	128.3	128.9
Cr VII	161.1	160.3	161.1
Mn VIII	196	195.4	196.1
Fe IX	235	233.8	234.7
Co X		275	(276)
Ni XI		320	(321)
Cu XII		367	(369)
Zn XIII		418	(420)
Ga XIV		471	(474)
Ge XV		528	(531)
As XVI		588	(591)
Se XVII		650	(654)
Br XVIII		716	(720)
Kr XIX		785	(789)

K Sequence:

The non-relativistic extrapolated values (beyond Fe VIII) are the uncorrected CFF energies. The corrections Δ_{CFF} are quite small.

Spectrum	E(EXPT)	E(CFF)
K I	4.340 eV	4.013 eV
Ca II	11.871	11.328
Sc III	24.76	24.61
Ti IV	43.25	43.35
V V	65.2	65.53
Cr VI	90.6	91.03
Mn VII	119.27	119.75
Fe VIII	151.6	151.7
Co IX		187
Ni X		225
Cu XI		266
Zn XII		311
Ga XIII		358
Ge XIV		409
As XV		462
Se XVI		519
Br XVII		579
Kr XVIII		642

Ca Sequence:

The non-relativistic extrapolated values (beyond Cr V) are the uncorrected CFF energies.

Spectrum	E(EXPT)	E(CFF)
Ca I	6.113 eV	5.320 eV
Sc II	12.80	12.225
Ti III	27.47	27.86
V IV	46.71	47.30
Cr V	73 ?	70.2
Mn VI		97
Fe VII		126
Co VIII		159
Ni IX		195
Cu X		234
Zn XI		276
Ga XII		321
Ge XIII		369
As XIV		421
Se XV		475
Br XVI		533
Kr XVII		593

Sc Sequence:

The non-relativistic extrapolated values (beyond Mn V) are the uncorrected CFF energies.

Spectrum	E(EXPT)	E(CFF)
Sc I	6.54 eV	5.72 eV
Ti II	13.58	13.00
V III	29.31	30.35
Cr IV	49.6	50.40
Mn V	76 ?	74.0
Fe VI		101
Co VII		131
Ni VIII		165
Cu IX		201
Zn X		241
Ga XI		284
Ge XII		330
As XIII		379
Se XIV		431
Br XV		486
Kr XVI		545

Ti - Ni Sequences:

The non-relativistic extrapolated values are the uncorrected CFF energies.

Spectrum	E(EXPT)	E(CFF)
Ti I	6.82 eV	6.01 eV
V II	14.65	15.90
Cr III	30.96	32.57
Mn IV		53.2
Fe V		77
Co VI		105
Ni VII		136
Cu VIII		170
Zn IX		207
Ga X		248
Ge XI		291
As XII		338
Se XIII		388
Br XIV		441
Kr XV		497

V Sequence:

Spectrum	E(EXPT)	E(CFF)
V I	6.74 eV	6.27 eV
Cr II	16.50	17.67
Mn III	33.67	35.05
Fe IV		56
Co V		81
Ni VI		110
Cu VII		141
Zn VIII		176
Ga IX		214
Ge X		255
As XI		300
Se XII		347
Br XIII		398
Kr XIV		451

Cr Sequence:

Spectrum	E(EXPT)	E(CFF)
Cr I	6.765 eV	6.307 eV
Mn II	15.640	15.011
Fe III	30.651	35.833
Co IV		57.52
Ni V		82.8
Cu VI		111
Zn VII		144
Ga VIII		179
Ge IX		217
As X		259
Se XI		304
Br XII		352
Kr XIII		403

Mn Sequence:

Spectrum	E(EXPT)	E(CFF)
Mn I	7.432 eV	6.745 eV
Fe II	16.182	15.35
Co III	33.50	37.17
Ni IV		59
Cu V		85
Zn VI		114
Ga VII		147
Ge VIII		183
As IX		222
Se X		264
Br XI		310
Kr XII		358

Fe Sequence:

Spectrum	E(EXPT)	E(CFF)
Fe I	7.90 eV	7.02 eV
Co II	17.06	19.99
Ni III	36.17	38.59
Cu IV		61
Zn V		87
Ga VI		117
Ge VII		151
As VIII		187
Se IX		227
Br X		270
Kr XI		316

Co Sequence:

Spectrum	E(EXPT)	E(CFF)
Co I	7.86 eV	7.28 eV
Ni II	18.15	20.93
Cu III	36.83	40.04
Zn IV		63
Ga V		90
Ge VI		120
As VII		154
Se VIII		191
Br IX		232
Kr X		275

Ni Sequence:

Spectrum	E(EXPT)	E(CFF)
Ni I	7.634 eV	7.517 eV
Cu II	20.291	22.04
Zn III	39.722	41.74
Ga IV	64.2	65.53
Ge V	93.4	93.02
As VI	127.5 ?	124.0
Se VII	155 ?	158
Br VIII	193 ?	196
Kr IX		237

Cu Sequence:

The non-relativistic extrapolated values (beyond Se VI) are the CFF energies with a ζ^2 correction added.

Spectrum	E(EXPT)	Uncorrected E(CFF)	I. P.
Cu I	7.726 eV	6.489 eV	7.726 eV
Zn II	17.964	16.64	17.964
Ga III	30.7	29.27	30.7
Ge IV	45.7	44.07	45.7
As V	62.6	60.9	62.6
Se VI	81.7	79.7	81.7
Br VII		100	(103)
Kr VIII		123	(125)

Zn - Ga Sequences:

The few unobserved values shown are the result of a ζ^2 extrapolation of the experimental data.

Ge - Kr Sequences:

All the values shown are experimental.

E(EXPT) in eV for the Zn - Kr Sequences:

	Spectrum Number I	II	III	IV	V	VI	VII
Zn	9.394	17.964	39.722	(63)	(87)	(114)	(144)
Ga	6.00	20.51	30.7	64.2	(90)	(117)	(147)
Ge	7.88	15.93	34.22	45.7	93.4	(120)	(151)
As	9.81	20.2	28.3	50.1	62.6	127.5	(154)
Se	9.75	21.5	32.0	42.9	73.1	81.7	155
Br	11.81	21.6	35.9	[48]	[61]	[96]	(103)
Kr	13.999	24.57	36.95	[53]	[67]	[82]	[123]

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13. ABSTRACT

The ionization potentials of the isoelectronic sequences Helium through Zinc have been calculated by the Hartree-Fock method and compared with experimental results. Tables are presented showing the ionization potentials, as observed and extrapolated, for all stages of ionization of the first 36 elements.

14 KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Ionization potentials						
Multiply-charged ions						
Isoelectronic sequence						
Hartree-Fock calculations						